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Scalable Coupling of Multi-Scale AEH and PARADYN Impact Analyses

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Abstract

This work describes scalable coupling of two stand alone computer codes for multi-scale impact analysis of composites. An asymptotic expansion homogenization (AEH) based micro-structural code available for modeling micro-structural aspects of modern armor materials is coupled with PARADYN, a parallel explicit Lagrangian finite element code. The first code enables modeling of material micro-structures in simple loading situations in stand alone form. The coupling of this code to PARADYN, which is a parallel version of the Lawrence Livermore National Laboratory (LLNL)'s serial DYNA3D, enables a micro-macro type multi-scale analysis of large elastic-plastic deformation response of structures under generalized three dimensional impact conditions. Three sets of results are presented to demonstrate: 1) the verification of the AEH-PARADYN model coupling to PARADYN, 2) validation of the AEH, and 3) the scalability of the coupled model.

1. Introduction

Spanning a composite from its micro-phases' level to its global structural level with finite elements lead to large meshes; the resulting computations are both expensive and intractable. Multi-scale analyses are used to alleviate this problem. At a basic level, these analyses express the micro-level response as a local perturbation of global response. While many theories are available for linking the micro-structural response to the global response, the AEH theory used in the first code is extended by Chung, Namburu, and Tamma, (1999) to armor composite impacts.

In the AEH approach, the micro-level response was expressed in terms of the global response in a strict, mathematically seamless approach. An updated Lagrangian scheme is employed to account for large displacements, strains, and rotations. At each time step, the equilibrium solution from the previous time step is used to update the local micro-structure. Since explicit time integrations take quite a large number of time steps and micro-level computations are to be performed at each and every time step, scalable computational approaches are needed to use this computationally intensive method. With the aid of domain decomposition and Message Passing Interface (MPI), the basic equations of Chung (1999) were re-cast for parallel computation and were shown to be scalable by Valisetty (2000) in a stand alone code. In the present work, this code is coupled to PARADYN within the message passing interface (MPI) scheme of the latter. Three sets of results are presented to demonstrate the verification, validation, and scalability of the AEH model coupling to PARADYN.

2. Coupling the AEH Model in PARADYN

PARADYN is a general purpose explicit dynamics code with a capability for defining multiple element types and material types. Each element of the global finite element model that is tabbed for detailed micro-level analysis is made to call the micro-structural AEH model to sample the local micro-level behavior and build the element global stresses from the constituent micro-stresses. The details of the coupling will be published in an ARL report.

2.1. Guidelines for using the Model.

The micro-structural AEH option can be specified by using a Type 3 material in PARADYN input and then additionally a non-zero number in the 5th data on the 8th material card of the material data input. The material option describes a non-linear elastic-plastic response with kinematic and/or isotropic hardening. The added micro-code is not limited to micro-phase materials of this type, however.

Micro-structure is next defined with the usual nodes, elements and material properties. Although any type of format can be used for this purpose, the one that is selected uses the same PARADYN input format. This was done to avail PARADYN pre-processors such as INGRID. Although not verified at present, there are no restrictions on the number of micro-structural elements, nodes and materials.

All the information defining the micro-structural AEH is to be contained in an input file separate from the PARADYN's global structure defining input file and is to be made available to the PARADYN executable along with a domain decomposition part file.

2.2. Details of the Data Exchange.

While PARADYN focuses on global computations such as the aggregation of nodal forces, solution of the equations of motion, updating global nodal positions, enforcing contact, etc., the micro-structural AEH code focuses on the micro-structural AEH calculations which typically involve evaluating the microstructure as a perturbation of global deformation and periodicity. For the respective codes to do their parts of computation, it is necessary that the relevant data be exchanged between them for each time step and for each global element identified for micro-computations. In the present work, the data exchange involved two parts as follows:

1. From PARADYN, at the beginning of each time step and for the identified global elements, the following data is written to external processor specific data files for read access to the micro-structural AEH model:

    current time step,
    current global strain increments,
    global strains from previous time step
    global stresses from previous time step
    effective plastic strain from previous time step

2. After reading the PARADYN written data files, micro-structural AEH computes and writes the following data to external processor specific data files for read access to PARADYN:

    Effective density
    Effective bulk modulus
    Effective shear modulus
    Computed current global stresses for the element
    Computed current effective plastic strain for the element

While PARADYN's native arrays are used for tracking global-stresses, global-strains, effective properties (density, bulk modulus, shear strain), and effective plastic strain, no such native arrays are used for the micro-element quantities. Instead these too are written to, and read from, processor specific files during each time step and updated during every time step.

As opposed to the global-stresses of the global elements, the stored values of these responses reflect the accurate stress distribution within the micro-elements of the microstructure. During a PARADYN run, or after the run is complete, the processor specific files can be visualized independently for observing the micro-structural stress and deformation development for any of the global elements.

3. Results

The following numerical analyses are conducted on the ARL's SGI O2k machines for verifying and validating the model's coupling and scalability.

3.1. Verification of the Model Coupling.

For verifying the model coupling, a small cylinder with homogeneous material was considered in a Taylor impact, and was analyzed alternatively as a homogeneous material with DYNA3D and as a homogeneous material with alternating layers of two different materials but with same identical properties using the micro-structural AEH in PARADYN. The idea was that the AEH model should default into a homogeneous material solution, and any discrepancy that shows up may point to errors in the data exchange in the codes' coupling.

Enforcing quarter symmetry on sides parallel to the axis of the cylinder, a 90 degree wedge of the cylinder was considered with 108 elements in five rows as shown in Figure 1. The length and radius of the cylinder are 2.592 mm and 3.2 mm, respectively. The material was considered elastic-plastic with isotropic hardening. The material properties are as follows:

Table 1. Material Properties

Density gm/mm^3	Young's modulus MPa	Poisson ratio	Yield stress MPa	Tangent modulus MPa
8.90E-03	117,000	0.35	4,000	1000

The velocity of the cylinder is 227 mm/ms. To cause the deformation, one end of the cylinder is assumed to be free of velocity. Results for axial velocity, axial stress and effective plastic strain are considered at the impacted end.

They are presented in Figures 2–4, respectively for the homorogeneous DYNA3D solution and for the homogeneous micro-structural AEH-PARADYN solution. Both solutions appear to be in agreement with each other thus verifying the model coupling for micro-structures with homogeneous materials.

3.2. Validation of the Model

In this example, a cylinder similar to the one in the previous example was considered but with two materials alternating in a total of 96 layers normal to the cylinder axis. The length and radius of the cylinder are 31.1 mm and 3.2 mm, respectively. The material was considered elastic-plastic with isotropic hardening. The material properties are as follows:

Table 2. Material Properties

Layer	Density kg/m^3	Young's modulus GPa	Poisson ratio	Yield stress GPa	Tangent modulus GPa
1	8930	1.17E+11	0.35	4.E+08	1.E+08
2	8930	9.00E+10	0.35	4.E+08	1.E+08

Two solutions were obtained. The first solution was a heterogeneous DYNA3D solution obtained using 10,368 global elements. To model the repeating 48 sets of the two dissimilar materials, 8 rows of elements were used for each material layer. The second solution was the homogeneous micro-structural AEH-PARADYN solution obtained with a 1,296 element global model. The elements are stacked in 96 layers. In contrast to the first solution, a single layer of elements was used for each material. All layers are assumed to be exhibiting homogeneous composite behavior in the global sense but with micro-structural AEH computed using a two layer micro-structural model.

Enforcing quarter symmetry on sides parallel to the axis of the cylinder, a 90 degree wedge of the cylinder was considered. The velocity imposed on all but one end face of the cylinder is 227 m/s. Figures 5 and 6 show the two models both before and after the impact.
Solutions at a node near the bottom of the cylinder are presented in Figures 7–9, for axial velocity, axial stress, and effective plastic strain.

For all these responses, the micro-structural AEH was able to track the DYNA3D's heterogeneous responses well. Deviations in the axial velocity and axial stress can be attributed to three factors: 1. these differences are near stress free edges prone to be affected by the transients; 2. the meshes are different in their coarseness which affects the time integration in the two solutions; and 3. the values are node averaged but the nodes are at different locations in the two models since the meshes are different. Similarly, the differences in the plastic strain predictions can be attributed to the extreme length of the time duration of the analysis which makes the differences to pile up.

3.3. Scalability of the Results.

As explained in Section 3.2, due consideration is given to the fact that PARDYN is a parallel code while coupling the micro-structural AEH. Since the PARADYN code has a well tested MPI/OPENMP based computational logic, the coupling was done by keeping a global element's micro-structural AEH computations local to the processor on which the global element resides. This means that information such as micro-element stresses, strains and mechanical properties needed in micro-element computations are kept local and not passed into global data structures. This means that a global element's micro-stress, micro-strain and micro-mechanical properties are needed to be written to, and read from, processor-specific files in between time steps. To underscore the fact that the penalty associated with this approach is small, results from a limited scalability study are presented in this section.

Taylor impact model of Section 4.2 is used for this purpose. Two types of scalability studies, one with a fixed mesh for standard scalability, and the other with varying mesh size, but with a fixed number of elements per processor, for scaled scalability are performed. The nodes, elements and wall clock times from these studies are presented next.

In these models, the increase in number of elements was achieved by adding element rows in the cylindrical axis direction only, and not in the hoop and radial directions.

The wall clock times are plotted in Figures 10 and 11. The plot in Figure 10 shows run times for the 122,880 element mesh for the standard scalability study. A linear scalability can be discerned from this plot.

On the other hand, the plot in Figure 11 shows the run times for the scaled scalability study. In this study, the mesh size was doubled with each doubling of the processors. The run times did not remain constant as were the number of elements per the processor. The reason could be that the plastic deformation is much more concentrated near base and the domain decomposition used to distribute the elements over the processors is not sensitive to this fact.

4. Future Work and Conclusions

Micro-structures are features of the US Army's advanced structures and armor materials. Homogenization theories such as the AEH are being developed to model the effect of these structures on global material and structural responses. With the present coupling of the AEH based micro-structural model in PARADYN, many in-situ material responses can be studied under diverse global structural conditions. The brief example applications presented in the presentation demonstrate this.

In future, the following extensions to this work will be considered: 1. using PARADYN's diverse material library to model the different micro-phase materials, 2. extending the application range to include complex micro structures and diverse global applications.

Acknowledgement

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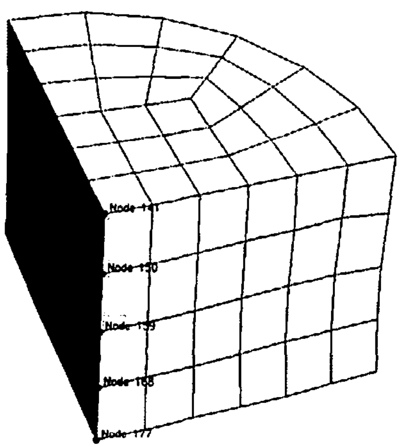

Figure 1. Finite element mesh of a cylindrical wedge under Taylor impact

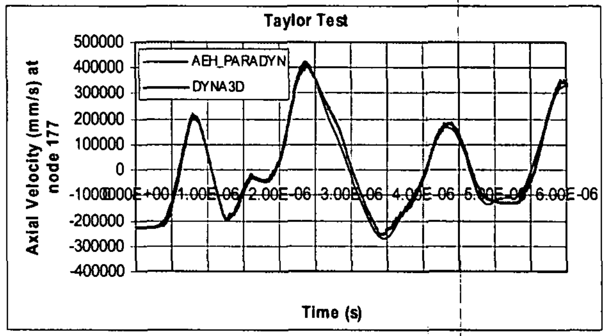

Figure 2. Axial velocity solutions for the finite element mesh of Figure 1

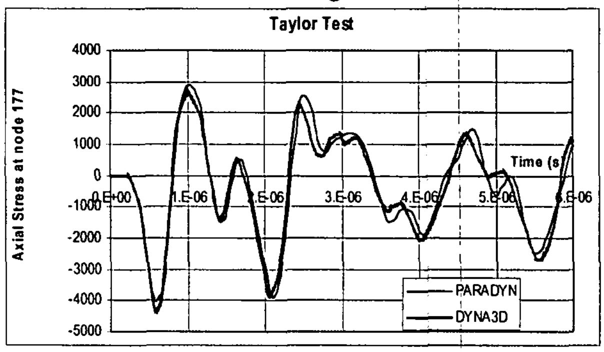

Figure 3. Axial stress solutions for the finite element mesh of Figure 1

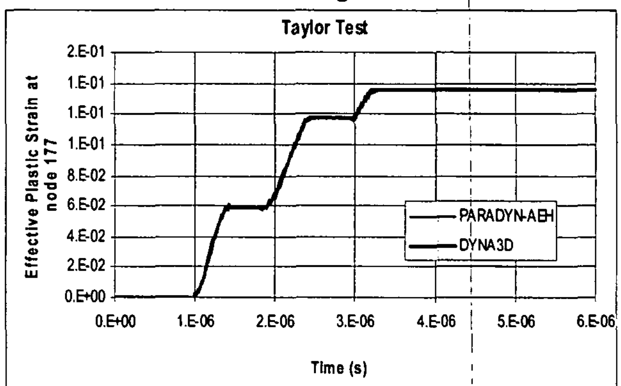

Figure 4. Effective plastic strain solutions for the finite element mesh of Figure 1

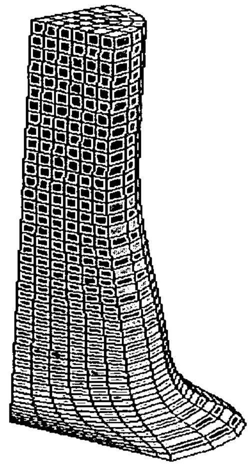

Figure 5. Finite element model and deformed mesh used for the AEH-PARDYN solution for the verification problem

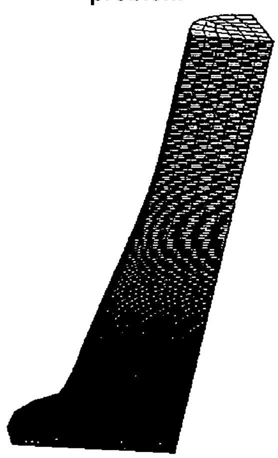

Figure 6. Finite element model and deformed mesh used for the DYNA3D solution for the verification problem

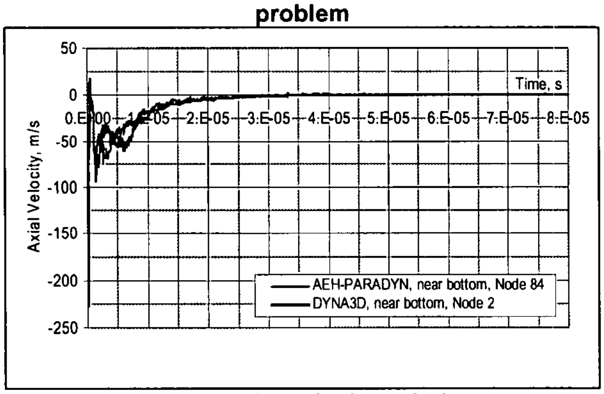

Figure 7. Axial velocity solutions

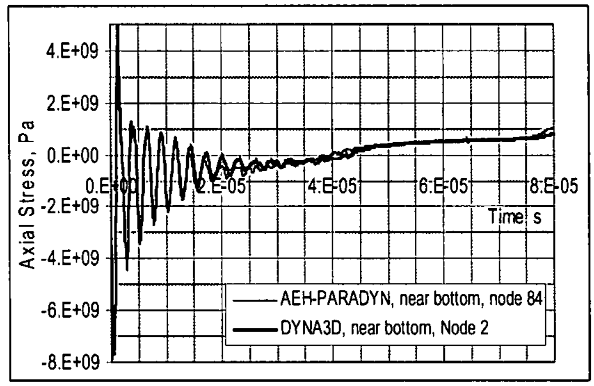

Figure 8. Axial stress solutions

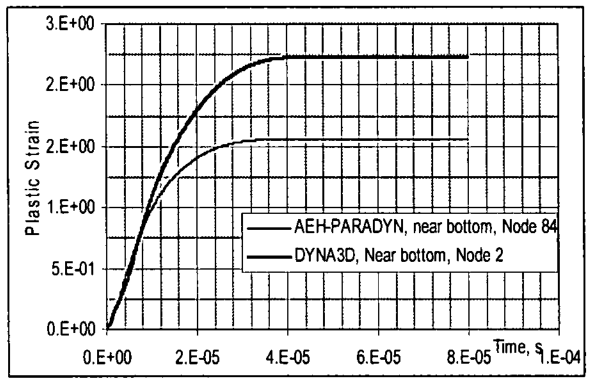

Figure 9. Effective plastic strain solutions

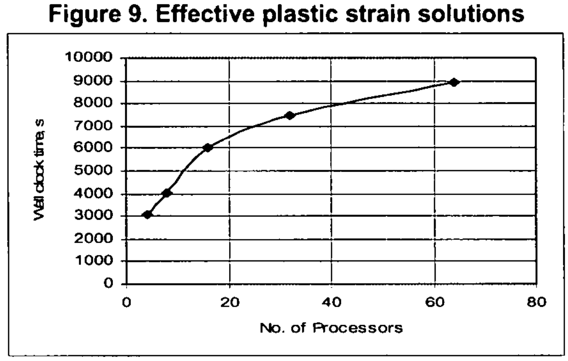

Figure 10. Linear Scalability Study

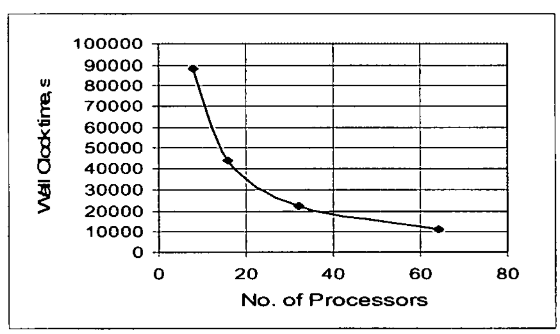

Figure 11. Scaled Scalability Study